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(54) Title: CRYSTAL LATTICE QUANTUM COMPUTER

(57) Abstract

A quantum computer comprises a crystal lattice having storage atoms. The storage atoms have nuclear storage spins, and quantum bits are stored as orientations of the storage spins. A magnetic field is applied to the crystal, the magnetic field having a gradient on the order of 1T/ μm . The gradient is generated by a micromagnet. The electrons of the crystal acquire a regular order and the storage spins are initialized by inducing combined electron-nucleus transitions in the crystal, thereby transferring the electronic order to the storage spins. The storage spins are decoupled from each other by a decoupling magnetic field. Quantum logic operations are performed on the storage spins. Certain quantum logic operations require a modification of the decoupling field to recouple a plurality of the storage spins. Final polarizations of the storage spins are measured.

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PCT Patent Application
for
Crystal Lattice Quantum Computer

Field of the Invention

This invention pertains generally to quantum computers, and in particular to a solid state
20 quantum computer comprising a crystal lattice.

Background

A quantum computer is a machine that prepares a quantum mechanical system in an initial input
25 state, performs unitary logic operations on the system, and measures a resulting output state. The
superposition principle of quantum mechanics and the quantum interference induced by a
projective measurement bring about "quantum parallelism," by which certain problems can be
computed faster than by any classical computer.

30 Several physical systems are known to provide the quantum mechanical states that carry
quantum bit, or "qubit," information. Each of these systems carries its own disadvantages. (i)
Cold trapped ions, cavity quantum electrodynamics, and combinations of the two systems allow
computation and final readout to be performed on individual qubits. However, these techniques
require immense experimental exertion. (ii) Single photon gates, compatible with quantum
35 communication links, are possible only in the presence of large optical nonlinearity with
negligible loss. (iii) Systems of nuclear spins in solution molecules are based on natural and
simple chemical structures and well-established techniques of pulsed nuclear magnetic
resonance. However, such systems demand a large number of molecules to detect the output

5 signals from slight population differences between nuclei with up spins and those with down spins. Furthermore, these liquid systems cannot be cooled to low temperatures to reduce thermal noise, since the liquids would freeze. (iv) Solid state systems can be used, including quantum dots, Josephson junctions, and nuclear spins of implanted phosphorous ions in silicon. However, these solid state systems would require technical breakthroughs before they could be scaled up to
10 large numbers of distinct qubits.

There is a need, therefore, for a quantum computer that does not require cumbersome experimental techniques, that can be cooled to low temperatures, and that can be scaled to large numbers of qubits.

15 A solid state crystal can be considered for quantum computation, wherein qubits are represented by spins of individual atoms or nuclei. However, it is not obvious how to distinguish between adjacent spins in the crystal, since the spins are so close together (on the order of 10 angstroms). Furthermore, spurious couplings among the atoms of the crystal will contaminate the quantum
20 computation.

Objects and Advantages

25 It is therefore a primary object of the present invention to provide a crystal lattice quantum computer wherein quantum bits are represented by nuclear spins, and adjacent spins can be distinguished. It is a further object of the present invention to cancel the spurious couplings within the crystal to reduce the error rate of the quantum computer.

30 The quantum computer of the present invention has the advantages that it has a relatively simple design, it can be cooled to low temperatures, and can be scaled up to include a large number of quantum bits.

Furthermore, the nuclear spins that store the quantum bits have a long relaxation time and are
35 isolated from their surrounding environment. The nuclei are regularly spaced in the crystal lattice, allowing them to be precisely addressed. The nuclei have spin-1/2, and have no isotopes with different nuclear spins. Finally, the nuclei are surrounded by localized electrons, allowing a magnetic order of the electrons to be utilized to initialize the nuclear spins efficiently.

5

Summary

A quantum computer comprises a crystal lattice having storage atoms. The storage atoms have nuclear storage spins. Quantum bits are stored as orientations of the storage spins. A magnetic field is applied to the crystal, the magnetic field having a gradient strong enough to cause energy levels of adjacent storage atoms along the direction of the gradient to be significantly different. The gradient is preferably created by a micromagnet in the vicinity of the crystal. The micromagnet preferably has a width on the order of $1\text{ }\mu\text{m}$ or less and generates a gradient on the order of $1\text{ T}/\mu\text{m}$. The micromagnet preferably comprises dysprosium.

15

The electrons of the crystal acquire a regular order. This order is utilized to initialize the storage spins as follows: combined electron-nucleus transitions are induced in the crystal, resulting in the transfer of the electronic order to the polarizations of the storage spins.

20

The storage spins are decoupled from each other by applying a time-varying decoupling magnetic field. The decoupling field eliminates spurious couplings that otherwise plague the crystal. The decoupling field rotates the storage spins in such a way as to cancel their magnetic dipole-dipole interactions. The decoupling field preferably comprises series of $\pi/2$ - pulses.

25

Quantum logic operations are performed on the storage spins. In a one-bit gate, a storage spin is rotated by an angle θ . A two-bit exclusive-OR gate involves the interaction of two storage spins. To carry out the exclusive-OR operation, the two storage spins must be recoupled by either modifying or switching off the decoupling field. The exclusive-OR operation is then achieved by applying an oscillating magnetic field to the crystal, wherein the oscillating magnetic field has a frequency equal to a resonance frequency of the recoupled storage spins.

30

Measurement of final polarizations of the storage spins is achieved by applying an oscillating measurement magnetic field to the crystal and measuring an amount of absorption of the measurement field. In the preferred embodiment, the crystal comprises measurement atoms, and the measurement field has a frequency equal to a resonant frequency of a coupled system comprising at least one measurement atom and at least one storage atom.

35

Brief Description of the Drawings

Fig. 1 shows a crystal used in a quantum computer.

Fig. 2 is an energy level diagram for electrons in the crystal.

Fig. 3A illustrates the quantum computer according to a preferred embodiment of the invention.

Fig. 3B shows a sample holder and a coil enclosing the crystal.

Fig. 3C shows an assembly comprising the crystal.

Fig. 4 is an energy level diagram for a combined nucleus-electron system of the crystal.

Figs. 5A and 5B illustrate pulse sequences used in a decoupling magnetic field.

Fig. 5C illustrates a pulse sequence used in a recoupling magnetic field.

Fig. 6 is an energy level diagram of a coupled system of two storage spins belonging to the crystal.

Detailed Description

I. Crystal

Fig. 1 shows a crystal 10 used in a quantum computer of the present invention. Crystal 10 comprises spectator atoms 14 and active atoms having non-zero nuclear spins. The active atoms comprise storage atoms 12. In the preferred embodiment, the active atoms also comprise measurement atoms 16. Measurement atoms 16 are preferably identical to storage atoms 12; the measurement atoms are distinguished from the storage atoms by their locations. This distinction is further discussed below.

For the purposes of illustration, only a few atoms appear in Fig. 1. However, crystal 10 in general comprises any number of atoms, such as one hundred million or more.

- 5 The atoms of crystal **10** preferably form a regular lattice. The nuclei of storage atoms **12** have storage spins **24**, and the nuclei of measurement atoms **16** have measurement spins **26**. Quantum bits, or qubits, are stored by storage spins **24**. In the preferred embodiment, storage spins **24** are spin-1/2, and storage atoms **12** do not have isotopes with other nuclear spins. Only five elements, ^{19}F , ^{31}P , ^{89}Y , ^{103}Rh , and ^{169}Tm , satisfy these requirements. Therefore, in the preferred
- 10 embodiment, storage atoms **12** and measurement atoms **16** are all either fluorine, phosphorus, yttrium, rhodium, or thulium.

In the preferred embodiment, storage atoms **12** and measurement atoms **16** form a salt structure with spectator atoms **14**. It is known that rare-earth elements form compounds known as "rare-

15 earth salts" with group VA elements, including phosphorous. In the embodiments where the measurement atoms are phosphorous, it is preferred that the spectator atoms are atoms of a rare-earth element. Among the rare-earth elements, cerium is the simplest, since a cerium atom has zero nuclear spin (all other rare-earth elements have nonzero nuclear spins).

- 20 Therefore, in the preferred embodiment, storage atoms **12** and measurement atoms **16** are phosphorous, and spectator atoms **14** are cerium. In a cerium monophosphide crystal, each cerium atom has only one unpaired 4f electron. Crystals of cerium monophosphide, or CeP , are now obtainable using recently developed crystal growth techniques; see Y.S. Kwon et al., *Physica B* 171 (1991) p. 324 and Y. Haga et al., *Physica B* 206 & 207 (1995) p. 792.

25 Cartesian x, y, and z axes are oriented as shown in **Fig. 1**, preferably with each of the axes normal to a face of crystal **10**. The z-axis points in a longitudinal direction, and the x- and y-axes point in lateral directions perpendicular to the longitudinal direction.

- 30 A static magnetic field **20** is applied to crystal **10**. The static magnetic field has a component in the z-direction. The crystal is preferably kept at a temperature below the Néel temperature, approximately 8.5K for CeP . In the preferred embodiment, when static magnetic field **20** is applied, a magnetic order is created among the electrons of spectator atoms **14**.

- 35 In the preferred embodiment, the spectator atoms are cerium atoms, and each cerium atom has a single unpaired 4f electron. The electron belongs to a ^2F multiplet, which is split by the spin-orbit interaction to produce a $^2\text{F}_{7/2}$ and a $^2\text{F}_{5/2}$ multiplet, see **Fig. 2**. The $^2\text{F}_{7/2}$ and $^2\text{F}_{5/2}$ multiplets

- 5 have an energy difference of approximately 280 meV, large enough that the higher energy $^2F_{7/2}$ levels can be ignored.

- A crystalline field present within crystal **10** splits the $^2F_{5/2}$ manifold into a Γ_8 quartet and a Γ_7 doublet, as shown in **Fig. 2**. The energy difference between the Γ_8 and Γ_7 multiplets is
10 approximately 15meV, an energy corresponding to a temperature of 170K. Because crystal **10** is kept at a low temperature (preferably less than 8.5K), the Γ_8 quartet can be ignored.

- Therefore each cerium atom of crystal **10** possesses an electron in the Γ_7 doublet, the eigenstates of which are written $|+\rangle$ and $|-\rangle$. The eigenstates $|+\rangle$ and $|-\rangle$ can be regarded as the eigenstates of
15 an effective spin operator. Therefore each cerium atom has an effective spin **22**, as shown in **Fig. 1**. Each of the effective spins is "up" or "down" (illustrated by a solid arrow pointing up or down in **Fig. 1**) depending on whether the corresponding electron is in the $|+\rangle$ state or the $|-\rangle$ state, respectively.

- 20 To reduce thermal excitations and thereby improve signal to noise in the quantum computer, crystal **10** is preferably kept at a temperature below 2K. Typically, crystal **10** has a temperature of 1K.

- When static magnetic field **20** has a magnitude on the order of 1 T or less, effective spins **22** of
25 the cerium atoms align in alternate α and β layers, as shown in **Fig. 1**. The layers are parallel to the xy-plane. In each α layer, the effective spins are up, and in each β layer, the effective spins are down.

- When static magnetic field **20** is applied, the nuclear spins of the active atoms (that is, storage
30 spins **24** and measurement spins **26**) couple to static magnetic field **20** via the Zeeman effect. The nuclear spins also couple to the effective spins of the neighboring electrons via the hyperfine interaction.

- Static magnetic field **20** has a magnitude in the z-direction equal to $B_z(x,y)$. When $B_z(x,y) < 1$
35 T, the effective spins acquire the anti-ferromagnetic order illustrated in **Fig. 1**, and the nuclear spins of the active atoms are described by two different Hamiltonians, one for the α layers and one for the β layers.

- 5 In each α layer, the storage spin 24 located at position (x,y) has a z-component I_z^α and an energy given by the following Hamiltonian:

$$H_\alpha = - (g_I \mu_N B_z(x,y) - A_{hf}^{iso} - 4 A_{hf}) I_z^\alpha \quad (1)$$

- 10 The first term in Eq. (1) gives the Zeeman splitting, the second gives the hyperfine splitting. The storage spin z-component I_z^α can take on values of +1/2 (up nuclear spin) or -1/2 (down nuclear spin). The constant g_I is the g-factor for the active atoms; in the preferred embodiment the active atoms are phosphorous and $g_I = 1.13$. The quantity μ_N is the nuclear magneton. The quantity A_{hf}^{iso} is the magnitude of an isotropic coupling, and has an experimentally determined value of
 15 approximately 4 MHz. The quantity A_{hf} determines the strength of the hyperfine interaction, and is given by:

$$A_{hf} = - (\mu_0/4\pi) g_I \mu_N g \mu_B / a^3$$

- 20 In this expression μ_0 is the permeability of free space; g is an effective g-factor for the effective spins and is equal to -10/7; μ_B is the Bohr magneton; and a is a lattice spacing of crystal 10, as shown in Fig. 1.

- In each β layer, the measurement spin 26 located at position (x,y) has a z-component I_z^β and an
 25 energy given by:

$$H_\beta = - (g_I \mu_N B_z(x,y) + A_{hf}^{iso} + 4 A_{hf}) I_z^\beta \quad (2)$$

- Eqs. (1) and (2) are similar, except for the signs in front of $4 A_{hf}$ and A_{hf}^{iso} , corresponding to
 30 opposite orientations of neighboring effective spins.

In the preferred embodiment, the active atoms in the α layers are storage atoms 12, and the active atoms in the β layers are measurement atoms 16. More generally, it is preferred that the storage atoms are a collection of atoms that have identical hyperfine energies.

- 35 In a second embodiment, the active atoms in the α layers are the measurement atoms, and the active atoms in the β layers are the storage atoms. In a third embodiment, all of the active atoms

are storage atoms, used for the storage and manipulation of quantum bits, regardless of their
hyperfine energies. In this third embodiment, there are no measurement atoms.

When the strength of static magnetic field **20** is larger than 1 T, the effective spins **22** in crystal
10 align themselves in a manner more complicated than the alternating sequence of Fig. 1. For
example, the effective spins may form several spin-up layers in a row, followed by a number of
alternating spin-up and spin-down layers. In the case of this and other complex magnetic order,
it is still preferred that the storage atoms all have the same hyperfine energies.

Although it is presently preferred that crystal **10** comprises CeP, other compositions of crystal **10**
are possible. In one embodiment, crystal **10** comprises CaF₂. This choice is advantageous
because most calcium atoms have no nuclear spin, and only a small percentage – 0.13% – have
spin 7/2. In another embodiment, crystal **10** comprises MnF₂. The MnF₂ crystal establishes an
anti-ferromagnetically ordered spin structure that has been well studied. In yet another
embodiment, crystal **10** comprises CeF₃. In these three embodiments, the storage atoms are
fluorine atoms. For more information on materials to be used for crystal **10**, see Thaddeus Ladd
et al., “Decoherence in Candidate Materials for Crystal Lattice Quantum Computation,” to be
published in Applied Physics A. More information on CeP can be found in F. Yamaguchi et al.,
“Crystal Lattice Quantum Computer,” Applied Physics A 68 (1999) 1-8.

II. Static Magnetic Field

Static magnetic field **20** points primarily in the z-direction. Static magnetic field **20** furthermore
has a gradient **21** in the x-direction, as illustrated in Fig. 1. Gradient **21** gives storage atoms **12**
different nuclear magnetic resonance frequencies, each resonance frequency depending upon the
x-coordinate of the associated storage atom.

In some embodiments, gradient **21** has a component in the x-direction but not in the y-direction.
In these embodiments, $B_z(x,y)$ is a function only of x , and is approximately uniform in planes
parallel to the yz -plane within crystal **10**. In other embodiments, the gradient **21** has components
both the x-direction and in the y-direction. In these embodiments, $B_z(x,y)$ is a function of both x
and y .

- 5 In general, gradient 21 points in any direction, including the z-direction. In the presently preferred embodiments, gradient 21 lies in the xy-plane, and the present discussion assumes that gradient 21 is perpendicular to the z-axis. This assumption, however, should not be construed as a limitation of the invention.
- 10 Fig. 3A illustrates a cutaway view of the quantum computer according to the preferred embodiment of the invention. A background magnetic field is generated by a magnet 34. Magnet 34 is preferably a superconducting magnet. A first coil 60 is resides within magnet 34. First coil 60 is connected to a first power supply 33.
- 15 Within first coil 60 is a second coil 62 which in turn encloses a sample holder 64, as shown in Fig. 3B. Second coil 62 is electrically connected to a second power supply 36 and to a signal processor 38. The first and second coils provide time-varying magnetic fields to crystal 10, as explained in detail below.
- 20 Inside sample holder 64 is an assembly 70, as shown in Fig. 3C. Assembly 70 comprises a micromagnet 30 attached to a substrate 32. Micromagnet 30 has a coating 31, to which is attached crystal 10.
- Micromagnet 30 is preferably ferromagnetic, and establishes a spatially varying magnetic field, thereby providing gradient 21. Magnetic field 20 is the sum of the magnetic field due to micromagnet 30 and the background field created by magnet 34.
- 25 Gradient 21 is preferably on the order of or greater than 1 T/ μm . This magnitude gives a difference in $B_z(x,y)$ of roughly 10^{-3}T between two adjacent storage atoms separated by 2a (approximately 12 angstroms). This difference corresponds to a Zeeman frequency difference of 8 kHz.
- For gradient 21 to have a value of 1 T/ μm or greater, micromagnet 30 must have a width w that is extremely small. In the preferred embodiment, width w is on the order of or less than 1 μm .
- 35 In some embodiments, width w is even smaller, taking on values on the order of 0.1 μm or even 0.01 μm .

- 5 To fabricate micromagnet 30 with the desired width, micromachining and deposition techniques are used. In the preferred embodiment, micromagnet 30 comprises dysprosium. In another embodiment, micromagnet 30 comprises cobalt.

- Coating 31 optimizes gradient 21 within crystal 10 by giving a spacing between micromagnet 30 and crystal 10. Coating 31 is preferably on the order of 1 μm thick. Coating 31 preferably comprises a polyamide.

- Assembly 70 causes gradient 21 to point in the x-direction. In another embodiment, assembly 70 comprises two side-by-side micromagnets in a "split gate" configuration. This configuration causes magnetic field 20 to vary in both the x- and y-directions. In alternate embodiments, gradient 21 is established by one or more current-carrying electrodes. More information on micromagnet 30 can be found in J.R. Goldman et al., "Magnet Designs for a Crystal Lattice Quantum Computer," to be published in Applied Physics A.

20

III. Initialization

- The qubits of the quantum computer are initialized by giving storage spins 24 initial polarizations. The initialization takes advantage of the Pound-Overhauser double resonance on the anti-ferromagnetically ordered effective spins and the nuclear spins. Storage spins 24 and measurement spins 26 are initialized by inducing combined electron-nucleus transitions in crystal 10.

- A total magnetic field in the α layers, $B_{\text{tot}}^{\alpha}(x,y)$ is the sum of static magnetic field 20 and an exchange magnetic field B_{exch} generated by the neighboring effective spins:

30

$$B_{\text{tot}}^{\alpha}(x,y) = B_z(x,y) + B_{\text{exch}}. \quad (3)$$

- Because of the anti-ferromagnetic structure of crystal 10, the β layers experience an exchange magnetic field in the opposite direction to that found in the α layers. Therefore a total magnetic field in the β layers $B_{\text{tot}}^{\beta}(x,y)$ is:

35

$$B_{\text{tot}}^{\beta}(x,y) = B_z(x,y) - B_{\text{exch}}. \quad (4)$$

- 5 The magnitude of B_{exch} is on the order of 10T.

As shown in Fig. 1, a storage spin at position (x,y,z) is surrounded by six effective spins 22, four of which are in the same xy-plane and two of which are located above and below the storage spin at locations $(x,y,z \pm a)$. Transition energies for the effective spins in the α layers is significantly different from transition energies for the effective spins in the β layers, primarily due to the different exchange magnetic fields, as given in Eqs. (3) and (4). Therefore, in considering the coupling of the storage spin at (x,y,z) to the effective spins in the β layers, the effective spins in the α layers can be ignored.

- 15 Fig. 4 shows an energy level diagram for the storage spin at position (x,y,z) and the effective spin immediately above the storage spin. The storage spin has z-component I_z^α , and the effective spin has z-component S_z^β . In a state A, both I_z^α and S_z^β equal $+1/2$; that is, both spins are up. In a state B, $(I_z^\alpha, S_z^\beta) = (+1/2, -1/2)$. States C and D are characterized by $(I_z^\alpha, S_z^\beta) = (-1/2, +1/2)$ and $(I_z^\alpha, S_z^\beta) = (-1/2, -1/2)$, respectively.

20 Transitions between states A and B, or between states C and D, are electron transitions. A combined electron-nucleus spin-flip transition 42 exists between states B and C. A transition between states A and D is not allowed.

- 25 At low temperatures, states B and D have roughly equal probabilities of being populated, and states A and C are unpopulated. To initialize the storage spin at (x,y,z) , an oscillating magnetic field B_1 having a frequency ω_1 is applied to crystal 10, wherein frequency ω_1 has a value necessary to induce combined electron-nucleus transition 42 from state B to state C. When the transition is induced, state C decays quickly to state D, leaving I_z^α in the down state.

30 Frequency ω_1 is given by:

$$\omega_1 = [|\mu_B| \mu_B (B_{\text{exch}} - B_z(x,y)) + g_N \mu_N B_z(x,y) - (3/2) A_{\text{hf}}^{50} - 3 A_{\text{hf}}] / \hbar. \quad (5)$$

- 35 In the above analysis, only the effective spin immediately above the storage spin at (x,y,z) was considered. An analysis of the coupling to the effective spin immediately below (x,y,z) shows that the oscillating magnetic field of frequency ω_1 can induce a combined electron-nucleus

- 5 transition involving the effective spin below (x,y,z) , again resulting in the storage spin being polarized in the down state.

Because frequency ω_1 depends upon $B_x(x,y)$, frequency ω_1 in general depends upon x and y . A plurality of oscillating magnetic fields having frequencies tuned according to the (x,y) locations of the storage atoms are applied. The oscillating magnetic fields cause the storage atoms and spectator atoms undergo combined electron-nucleus transitions that place substantially all of the storage spins into the down state.

- Similarly, the measurement atoms at (x,y) are polarized by applying an oscillating magnetic field B_{12} having frequency ω_2 , wherein

$$\omega_2 = [|g| \mu_N (B_{\text{exch}} + B_x(x,y)) - g_I \mu_N B_x(x,y) - (3/2) A_{\text{hf}}^{\text{iso}} - 3 A_{\text{hf}}] / \hbar. \quad (6)$$

- The result of applying B_{12} is to polarize the measurement atoms at (x,y) in the up state.
- 20 Oscillating magnetic fields B_1 and B_{12} are generated by first coil 60 in Fig. 3A.

In general, the storage spins are given initial directions, or polarizations, by inducing combined electron-nucleus transitions in crystal 10. This is true even when the electronic structure is different from the anti-ferromagnetic structure of the effective spins illustrated in Fig. 1. In some embodiments, the combined electron-nucleus transitions occur at optical frequencies.

IV. Decoupling

- Storage spins 24 are grouped into collections, wherein all of the storage spins in a given computation collection experience the same magnetic field $B_x(x,y)$. That is, magnetic field 20 has the same strength at each storage spin 24 in a given collection.

For example, when gradient 21 lies in the x -direction, the storage atoms in each collection lie in a plane parallel to the yz -plane. When $B_x(x,y)$ depends on both x and y , then each collection comprises storage atoms that lie in a line parallel to the z -axis.

- A time-varying decoupling magnetic field is applied to crystal 10 to decouple the storage spins from each other. The purpose of the decoupling field is twofold. First, the decoupling field eliminates interactions between storage spins within the same collection. This allows the storage

- 5 spins within each collection to act independently, and results in multiple parallel quantum calculations that do not interfere with each other.

The second purpose of the decoupling field is to decouple the different collections from each other. That is, the decoupling field also decouples storage spins having different locations along the direction of gradient **21**. This prevents the qubits represented by the storage spins in different collections from interfering with each other. When a quantum logic operation is to be performed on more than one collection, the relevant collections are recoupled during the operation. Quantum logic operations are further discussed below.

- 15 For the purposes of illustration, three storage spins are considered, and gradient **21** is parallel to the x-axis. A first storage spin I_1 is the nuclear spin of the storage atom at coordinates (x_1, y_1, z_1) . A second storage spin I_2 is the nuclear spin of a storage atom at coordinates (x_1+2a, y_1, z_1) . A third storage spin I_1' is the nuclear spin of a storage atom at coordinates (x_1, y_1, z_1+2a) . In this illustration, spins I_1 and I_1' belong to the same collection; spins I_1 and I_2 belong to different collections.
- 20

In the preferred embodiment, the decoupling magnetic field comprises a first series of pulses **52** and a second series of pulses **54**, as shown in **Figs. 5A** and **5B**. P_x and P_y are $\pi/2$ pulses about the x- and y-axes, respectively. \bar{P}_x and \bar{P}_y are $\pi/2$ pulses about the negative x- and negative y-axes, respectively. A time interval T characterizes the timing of the pulses. The pulses separated by T or by $2T$, as shown in **Fig. 5A**. T is typically on the order of 10 μsec .

25

First series **52** comprises $\pi/2$ pulses adjusted to operate on all storage spins having the same x-coordinate as I_1 . By applying the first series to crystal **10**, spins I_1 and I_1' are decoupled. This decoupling can be demonstrated by noting that the interaction Hamiltonian between spins I_1 and I_1' is proportional to $3 I_{1z} I_{1'z} - I_1 \cdot I_1'$, the average of which is zero under the influence of the first series.

30

Second series **54** is shown in **Fig. 5B**. The second series is a series of $\pi/2$ pulses, the duration and frequency of which have been adjusted to operate on storage spins having x-coordinate equal to x_1+2a . The interaction Hamiltonian between I_1 and I_2 is proportional to $I_{1z} I_{2z}$. Under the influence of series **52** and series **54**, the average interaction between I_1 and I_2 is zero. Therefore the decoupling field comprising the first and second series decouples the storage spins I_1 , I_1' , and

- 5 I₂. In the preferred embodiment, crystal 10 comprises measurement atoms 16, and the decoupling magnetic field also comprises components that decouple the measurement atoms from the storage atoms and from each other.

If it is desired to carry out a quantum logic operation on storage spins I₁ and I₂, the spins are recoupled. This recoupling is accomplished by applying a recoupling magnetic field to crystal 10. The recoupling field comprises first series 52 and a third series of pulses 56, illustrated in Fig. 5C. The recoupling field maintains the decoupling of spins I₁ and I₁' within the same collection, but couples the spin I₁ with the adjacent spin I₂.

- 15 Other decoupling and recoupling schemes are used in other embodiments of the invention. In one alternate embodiment, the decoupling magnetic field comprises a sequence of π -pulses to spin I₁, flipping the spin back and forth rapidly enough that it has no time-averaged effect on spin I₂.
- 20 In another alternate embodiment, the decoupling magnetic field comprises a sequence of two alternating magnetic fields parallel to the x-axis, each applied for a time T₁. The first alternating field rotates the storage spins located at (x,y) by an angle $\theta_1(x,y)$. The second alternating field differs from the first by a phase of π , and rotates the storage spins at (x,y) back to their original positions. Because static magnetic field 20 varies with x, angle $\theta_1(x,y)$ varies with x, and the
- 25 average interaction between I₁ and I₂ is zero. In the alternate embodiments above, the spins I₁ and I₂ are recoupled by temporarily switching off the decoupling magnetic field.

V. Quantum Logic Operations

- All quantum logic operations on an arbitrarily large number of qubits can be built up from one-bit gates and two-bit exclusive-OR gates. These operations can be performed as follows.

(a) One-bit gate:

An ith storage spin I_i is rotated by an angle θ . To accomplish this rotation, an alternating magnetic field B_q is applied along the x-axis for a time duration τ given by: $(g_i \mu_B B_i / \hbar) \tau = \theta$.

- 35 The magnetic field B_q has a frequency ω_q chosen to satisfy the resonance condition determined by Eq. (1).

(b) Exclusive-OR gate:

5 A two-bit exclusive-OR operation is performed on i^{th} storage spin I_i and an adjacent storage spin I_{i+1} , located a distance $2a$ along the x-axis from storage spin I_i . The exclusive-OR operation flips spin I_i only when I_{i+1} has a predetermined value, or flips I_{i+1} only when I_i has a predetermined value.

10 The z-components of the storage spins I_i and I_{i+1} are m_i and m_{i+1} , respectively. Neglecting interactions with other storage spins, the energy of storage spin I_i is: $E_i = \hbar \omega_i m_i$, where ω_i can be calculated from Eq. (1). Storage spins I_i and I_{i+1} are recoupled, either by using the recoupling field as outlined above, or by shutting off the components of the decoupling field that decouple spins I_i and I_{i+1} . The storage spins then form a coupled system with energy levels given by:

15

$$E = \hbar\omega_i m_i + \hbar\omega_{i+1} m_{i+1} + A_{nd}^1 m_i m_{i+1} \quad (7)$$

In Eq. (7), the term A_{nd}^1 gives a nuclear dipole interaction between storage spins I_i and I_{i+1} . In the preferred embodiment, where crystal **10** comprises CeP, A_{nd}^1 can be calculated from $A_{nd}^1 = (\mu_0/4\pi) (g_i \mu_N)^2/(2a)^3$, and has a value of 120 Hz.

20

The coupled system described by Eq. (7) is illustrated in Fig. 6. States G, H, I, and J correspond to $(m_i, m_{i+1}) = (-1/2, +1/2)$, $(+1/2, +1/2)$, $(-1/2, -1/2)$, and $(+1/2, -1/2)$, respectively. The energies of the states can be computed from Eq. (7). The corresponding resonant frequencies for transitions of the coupled system are given in Fig. 6.

25

To operate the exclusive-OR gate, an oscillating magnetic field B_0 is applied for a length of time suitable to provide a π -pulse. B_0 has a frequency equal to one of the resonant frequencies for a single spin-flip transition in the system of Fig. 6.

30

For example, when a π -pulse at frequency $\omega_i + A_{nd}^1/2\hbar$ is applied, spin I_i flips only when $m_{i+1} = +1/2$. A π -pulse at frequency $\omega_i - A_{nd}^1/2\hbar$ flips spin I_i only when $m_{i+1} = -1/2$. Similarly, π -pulses at frequencies $\omega_{i+1} \pm A_{nd}^1/2\hbar$ conditionally flip I_{i+1} .

35 (c) Other operations:

Other quantum logic operations are possible. Two qubits can be swapped as follows. In the coupled system of I_i and I_{i+1} represented in Fig. 6, a π -pulse is applied at frequency $\omega_i - \omega_{i+1}$.

- 5 After this pulse is applied, m_i is equal to the value that m_{i+1} had before the pulse; similarly m_{i+1} is equal to the prior value of m_i .

Another quantum logic operation is a three-bit exclusive-OR gate. Storage spins I_{i-1} , I_i , and I_{i+1} are three consecutive storage spins that lie in a line parallel to the x-axis. The three storage spins
 10 I_{i-1} , I_i , and I_{i+1} are coupled together to form a three-spin system. The three-spin system has energies:

$$E = \hbar\omega_{i-1}m_{i-1} + \hbar\omega_im_i + \hbar\omega_{i+1}m_{i+1} + A_{nd}^I m_{i-1}m_i + A_{nd}^I m_im_{i+1},$$

- 15 neglecting the dipole coupling between I_{i-1} and I_{i+1} . A π -pulse at a frequency $\omega_i + A_{nd}^I/\hbar$ flips storage spin I_i only when $m_{i-1} = m_{i+1} = 1/2$. π -pulses at frequencies $\omega_{i-1} + A_{nd}^I/2\hbar$ and $\omega_{i+1} + A_{nd}^I/2\hbar$ flip spins I_{i-1} and I_{i+1} , respectively, only when $m_i = 1/2$.

When a quantum logic operation operates on storage spin I_i having coordinates (x_i, y_i, z_i) , the
 20 quantum logic operation generally acts on all of the storage spins experiencing the same strength of magnetic field **20**. Therefore in general, quantum logic operations do not operate only on single storage spins, but on the collections of spins. Because the collections of atoms undergo quantum logic operations, and the atoms in each collection are decoupled, the quantum computer performs the same computation many times simultaneously.

25

VI. Measurement

The storage spins are first initialized. Then quantum logic operations are performed on the storage spins. As a final step in the process of quantum computation, final z-components, or
 30 polarizations, of the storage spins are measured. The measurement can be carried out in at least two ways.

Method 1: Nuclear Magnetic Resonance.

- The measurement atoms are preferably decoupled from the storage atoms by the decoupling magnetic field. To measure the final polarization of storage spin $I^a(x, y, z)$ of the storage atom at
 35 (x, y, z) , storage spin $I^a(x, y, z)$ is coupled to measurement spin $I^b(x+a, y, z+a)$. Because of the uniformity of magnetic field **20** in the z-direction, measurement spin $I^b(x+a, y, z+a)$ is thereby also coupled to storage spin $I^a(x, y, z+2a)$.

5

The three spins $I^a(x,y,z)$, $I^b(x+a,y,z+a)$, and $I^c(x,y,z+2a)$ form a coupled measurement system. To make a measurement, an oscillating magnetic measurement field B_m is applied to crystal 10, the frequency of B_m being equal to one of the resonant frequencies of the measurement system.

10 The Hamiltonian describing the interactions of the measurement system is:

$$H = - [g_I \mu_N B_z (x+a,y) + A_{hf}^{iso} + 4A_{hf}] I_z^b(x+a,y,z+a) - (1/2) A_{nd}^0 [I_z^a(x,y,z) + I_z^c(x,y,z+2a)] I_z^b(x+a,y,z+a) \quad (8)$$

15 Here A_{nd}^0 gives the nuclear dipole interactions between the measurement nuclei and the storage nuclei. $A_{nd}^0 = 2^{3/2} A_{nd}^1$, approximately 340 Hz for CeP.

When measurement field B_m has a frequency $[g_I \mu_N B_z (x+a,y) + 4A_{hf} + A_{hf}^{iso} + A_{nd}^0]/\hbar$ and is absorbed, the result of the measurement is that $I_z^a(x,y,z) = I_z^c(x,y,z+2a) = 1/2$. Similarly, when measurement field B_m has a frequency $[g_I \mu_N B_z (x+a,y) + 4A_{hf} + A_{hf}^{iso} - A_{nd}^0]/\hbar$, and is absorbed, the final polarizations of the storage atoms were $I_z^a(x,y,z) = I_z^c(x,y,z+2a) = -1/2$. Therefore the coupling of the measurement atoms with the storage atoms affords a measurement of the z-components of the storage spins.

25 To carry out the measurement, measurement field B_m is generated by second coil 62, as shown in Fig. 3B. Second coil 62 is connected to signal processor 38, which determines the amount of power lost to crystal 10 by second coil 62. That is, signal processor 38 determines the amount of absorption (if any) of measurement field B_m by crystal 10. From the absorption measurement, the final polarizations of the storage spins determined.

30

Method 2: Electron Spin Resonance.

The second method does not use the measurement atoms. This method uses the fact that the electron resonance of an electron at $(x,y,z+a)$ with effective spin S^B occurs at a frequency $[|g| \mu_B (B_{exch} - B_z(x,y)) + A_{hf}^{iso}/2 - A_{hf}]/\hbar$ if $I_z^a(x,y,z) = 1/2$, and at a frequency $[|g| \mu_B (B_{exch} - B_z(x,y)) - A_{hf}^{iso}/2 + A_{hf}]/\hbar$ if $I_z^a(x,y,z) = +1/2$. It is therefore possible to again measure the absorption of measurement field B_m having one of the above frequencies to determine the value of $I_z^a(x,y,z)$.

35

5 **VII. Further Considerations**

In the quantum computer of Figs. 3A – 3C, various time-varying magnetic fields are generated. In the presently preferred embodiment, the oscillating magnetic field B_i that initializes the storage spins is generated by first coil 60. The decoupling magnetic field, the oscillating
10 magnetic fields B_d and B_o that perform quantum logic operations, as well as the measurement field B_m are all generated by second coil 62. In general, any desired magnetic field generators may be used.

Although the above description contains many specificities, these should not be construed as
15 limiting the scope of the invention but as merely providing illustrations of some of the presently preferred embodiments of this invention. Thus the scope of the invention should be determined by the following claims and their legal equivalents.

Claims

We claim:

1. A method of performing a quantum computation, said method comprising the following steps:
 - a) applying a static magnetic field to a crystal, wherein:
said static magnetic field has a component along a longitudinal direction,
and said static magnetic field has a gradient;
and wherein
said crystal comprises a plurality of storage atoms, wherein the nucleus of
each of said storage atoms has a storage spin;
 - b) giving said storage spins initial polarizations by inducing combined nucleus-electron transitions in said crystal;
 - c) applying a time-varying decoupling magnetic field to said crystal, thereby decoupling said storage spins from each other;
 - d) performing a quantum logic operation in said crystal, wherein said quantum logic operation operates on a first of said storage spins; and
 - e) measuring a final polarization of at least one of said storage spins.
2. The method of claim 1, wherein said step of performing said quantum logic operation comprises the following step: rotating said first storage spin by an angle θ .
3. The method of claim 1, wherein said step of performing said quantum logic operation comprises the following steps:
 - a) recoupling said first storage spin with a second of said storage spins, thereby creating a coupled system comprising said first and second storage spins; and
 - b) applying an oscillating magnetic field to said crystal, said oscillating magnetic field having a frequency equal to a resonant frequency of said coupled system.

5

4. The method of claim 1, wherein said crystal further comprises a plurality of measurement atoms, wherein the nucleus of each of said measurement atoms has a measurement spin; and wherein said step of measuring said final polarization comprises the following step:

10

applying an oscillating magnetic field to said crystal, said oscillating magnetic field having a frequency equal to a resonant frequency of a coupled system comprising at least one of said storage spins and a first of said measurement spins.

15

5. The method of claim 1, wherein said quantum logic operation operates on a collection of said storage spins, wherein said static magnetic field has the same strength at each of said storage spins in said collection.

20

6. The method of claim 1, wherein said gradient is greater than 1 T/ μm .

7. The method of claim 1, wherein said crystal has a temperature of less than 2 K.

8. The method of claim 1, wherein said storage spins are spin-1/2.

25

9. The method of claim 8, wherein said storage atoms are selected from the group consisting of: fluorine, phosphorus, yttrium, rhodium, and thulium.

10. The method of claim 9, wherein said crystal comprises cerium monophosphide.

30

11. A quantum computer comprising:

- a) a crystal comprising a plurality of storage atoms, wherein the nucleus of each of said storage atoms has a storage spin;
- b) a means for generating a static magnetic field, wherein said static magnetic field has a component along a longitudinal direction, and said static magnetic field has a gradient;

35

- 5 c) a means for inducing combined electron-nucleus transitions in said crystal, for giving said storage spins initial polarizations;
- d) a means for generating a time-varying decoupling magnetic field, for decoupling said storage spins from each other;
- 10 e) a means for generating an oscillating magnetic field, for performing a quantum logic operation in said crystal, wherein said quantum logic operation operates on a first of said storage spins;
- f) a means for applying an alternating measurement magnetic field to said crystal; and
- 15 g) a means for detecting an absorption by said crystal of said measurement magnetic field.
12. The quantum computer of claim 11, wherein said quantum logic operation rotates said first storage spin by an angle θ .
- 20 13. The quantum computer of claim 11, wherein said oscillating magnetic field has a frequency equal to a resonant frequency of a coupled system comprising said first storage spin and a second storage spin.
- 25 14. The quantum computer of claim 11, wherein said crystal further comprises measurement atoms, wherein the nucleus of each of said measurement atoms has a measurement spin; and wherein said alternating measurement magnetic field has a frequency equal to a resonant frequency of a coupled system comprising at least one of said storage spins and a first of said measurement spins.
- 30 15. The quantum computer of claim 11, wherein said quantum logic operation operates on collection of said storage spins, wherein said static magnetic field has the same strength at each of said storage spins in said collection.
- 35 16. The quantum computer of claim 11, wherein said means for generating said static magnetic field comprises a micromagnet having a width of less than 1 μm .
17. The quantum computer of claim 16, wherein said micromagnet comprises a material selected from the group consisting of: dysprosium and cobalt.

5

18. The quantum computer of claim 11, wherein said storage atoms are selected from the group consisting of: fluorine, phosphorous, yttrium, rhodium, and thulium.

10

19. The quantum computer of claim 18, wherein said crystal comprises cerium monophosphide.

20. The quantum computer of claim 11, wherein said crystal has a temperature of less than 2K.

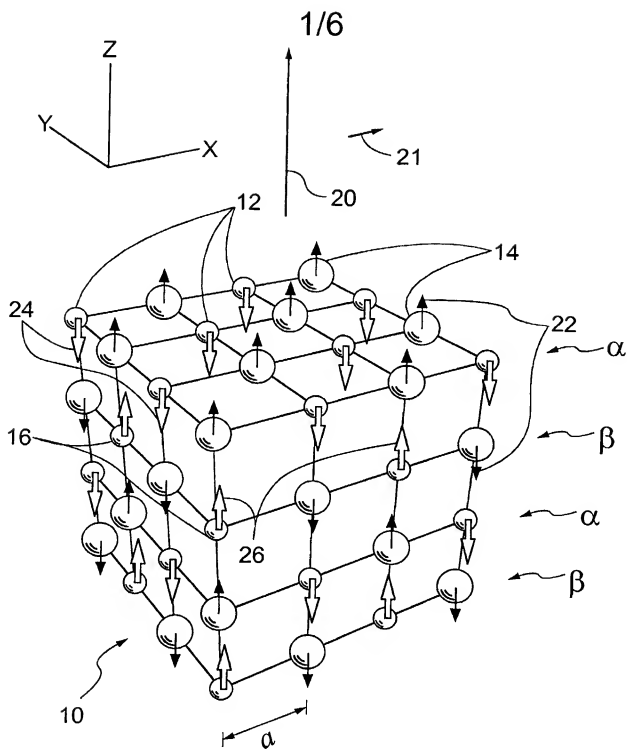


FIG. 1

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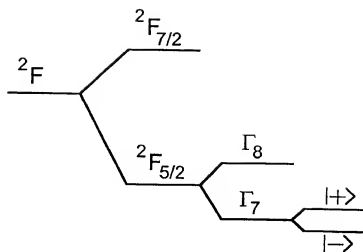


FIG. 2

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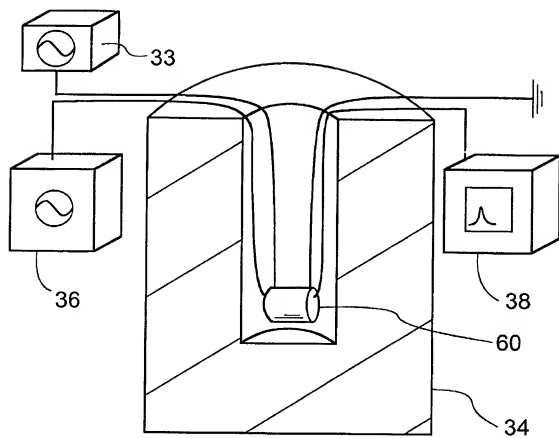


FIG. 3A

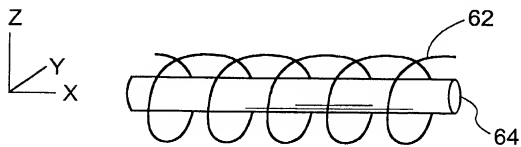
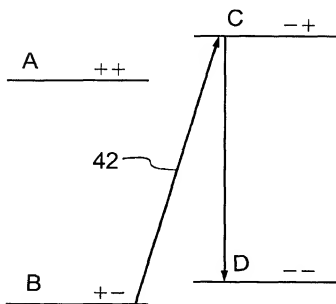
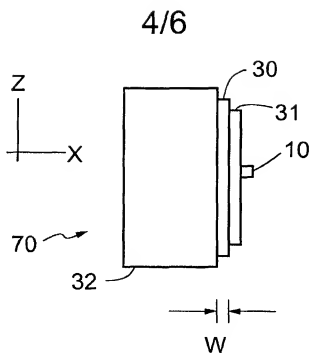


FIG. 3B



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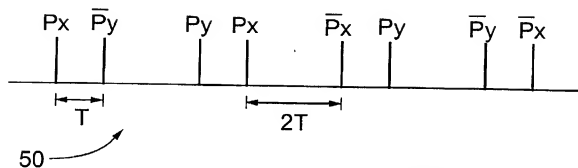


FIG. 5A

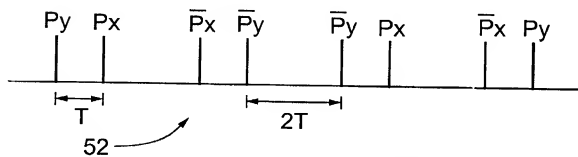


FIG. 5B

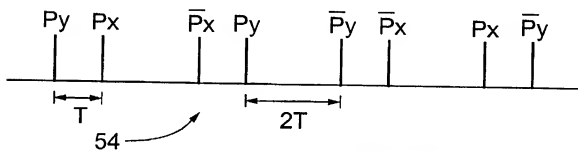


FIG. 5C

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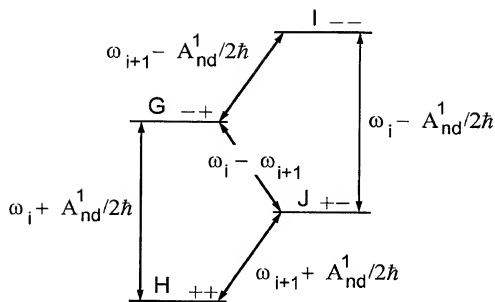


FIG. 6